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Deep level studies of GaN by deep level transient spectroscopy

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Abstract : Deep level studies of undoped, lightly-doped and moderately-doped GaN have been done, the dopant being Mg. An energy level of L_1 = 0.25 eV has been observed in all three types of samples and is considered to be due to unintentional dopant/impurity present in the grown sample. The concentration of this L_1 level is independent of doping level. Another level L_3 = 0.62 eV has been observed in lightly-doped and moderately-doped samples. The concentration of this L_3 level depends on the doping concentration and is considered to be due to Mg dopant. Another broad energy level L_2 has been observed only in lightly-doped sample but does not appear in undoped and moderately-doped sample. The broadening and peak height of this L_2 level are attributed to the contribution of more than one deep level. The origin and disappearance of this L_2 level in undoped and moderately-doped sample is not clear.

Keywords Deep level, activation energy, trap density, GaN

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1. Introduction

GaN is of wurtzite structure and has a direct band gap of 3.4 eV at room temperature. Undoped GaN is of *n*-type. Recently, development of efficient blue LEDs [1-4] and high temperature and high power electronics using GaN, has shown rapid progress. Moreover, there are reports of metal semiconductor FET [5], photodetector [6] and UV sensor [7] using GaN. Both Zn and Mg have been used as acceptors for a long time. The dramatic changes came when high quality *n*-type films and especially *p*-type GaN by doping Mg [1, 2, 8] were successfully achieved, although efforts of making *p*-type GaN by doping both Mg and Zn started long time back [9].

Deep levels in *n*-GaN are prime suspects in limiting the behaviour of GaN-based and other devices [10], especially the light emitting diodes (LEDs) and laser diodes (LDs). Therefore, a detailed study on deep levels of undoped and acceptor-doped GaN has become an acute need. In this paper, we present the deep level studies on undoped, lightly-doped and moderately-doped GaN where Mg is the dopant.

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2. Experimental

Epitaxial layers of GaN were grown by Metalorganic Vapour Phase Epitaxial (MOVPE) on (0001) sapphire substrate at about 1090°C. Prior to the growth, a thin AlN buffer layer (500Å) is deposited on the substrate at about 580°C. Trimethyl gallium (TMG), trimethyl aluminium (TMA) and NH_3 as source materials, were fed to the substrate with an ambient H_2. Biscyclopentadienyl (Cp_2Mg) of six-nine purity was used as precursor for Mg doping. *p*-type GaN by doping Mg was successfully achieved. The thickness of the grown layer was about 2 to 3 μm.

Au and Al of 5N purity were evaporated onto GaN at 10^{-6} torr as Schottky and ohmic contacts, respectively. It has been reported that Al forms good ohmic contacts and does not form any barrier with GaN [1, 11-14]. Therefore, we selected Al for the ohmic contact. The size of the Schottky contact was 3.71 × 10^{-4} cm^2. The value of the series resistance of the diode was observed to be about 120 ohm. These values are almost same in case of undoped samples and increases slightly with the increase of doping concentration. The Hall effect was measured for several samples at RT by using Van der Pauw method. The highest mobility achieved was 600 cm^2/V-sec in one of the undoped samples. The C–V measurement was also done at RT and ($N_D - N_A$) values derived from C–V measurement of typical samples are shown in Table 1.

Table 1. Activation energy, trap density and capture cross section of each levels in undoped samples, lightly-doped samples and moderately-doped samples

Sample	$N_D - N_A$ (cm^{-3})	Activation energy (eV)	Trap density (10^{13} cm^{-3})	Capture cross section (10^{-15} cm^2)
Undoped GaN	10^{16}	L_1 : 0.25±0.02	1.7	1.5
Lightly-doped GaN	8.9×10^{16}	L_1 : 0.25±0.02	1.8	3.3
		L_3 : 0.62±0.02	2.2	2.3
Moderately-doped GaN	9.2×10^{17}	L_1 : 0.25±0.02	1.7	2.7
		L_3 : 0.62±0.02	2.1	6.4

Under thermal equilibrium and in vacuum of 10^{-6} torr, the sample was cooled down to 77 K. Carriers are first injected by a forward bias of 3.5 volt, the duration of injection being 100 msec. Then, with the increase of temperature at a constant rate of 0.05 K/sec, the transient capacitance under a reverse bias of -4 volt was measured within a duration of 4000 msec corresponding to an applied sequence of positive pulse of 3.5 volt, where $C(t_n)$, n = 1, 2, ... 5 are the capacitances after 75, 225, 375, 675 and 1125 msec, respectively as shown in Figure 1. The values of $C(t_n)$ are read by LCR meter and are fed to the microcomputer. The Deep Level Transient Spectroscopy (DLTS) signal was processed by the computer using an exponentially decaying curve as a weighting function. The values of continuously varying temperatures of the sample are measured by digital voltmeter and also are fed to the microcomputer. The measurement of DLTS in the temperature range of 77 K to 400 K was carried out with HP multi-frequency LCR meter (model 4274 A), operated at 10 KHz.

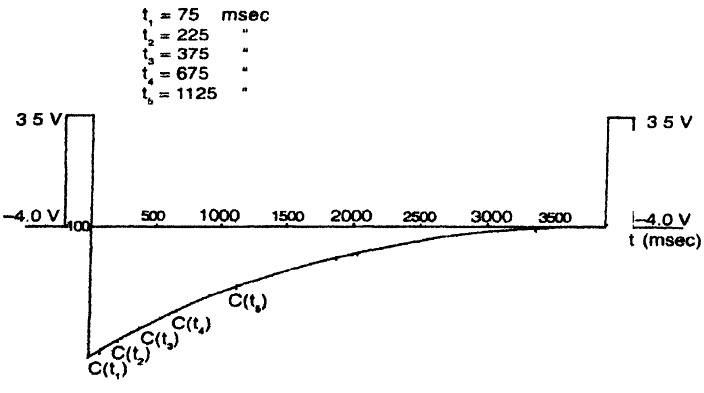

Figure 1. Transient capacitance measurement under a reverse bias of 4 Volt after an injection by a forward bias of 3.5 Volt was measured within a duration of 4000 m sec. For details, please see the text

In the DLTS mode of operation, the fixed value of the ratio of t_1/t_2 was maintained while the values of t_1 and t_2 were varied. The change in capacitances under a constant time ratio of 1/3 are (1) $S_1 = C(t_2) - C(t_1)$, (2) $S_2 = C(t_4) - C(t_2)$ and (3) $S_3 = C(t_5) - C(t_3)$.

Trap densities N_T were calculated using the expression [9]

$$N_T = N_A[\Delta C/C(V)]\left[1-\{2W_e/W(V)\}\{1-C(V)/C(0)\}\right.$$
$$\left.-\{C(V)/C(0)^2\}\right]^{-1},$$

where N_A is the free carrier concentration of GaN film, ΔC is the change in capacitance at $t = 0$, $C(0)$ is the steady state capacitance with zero bias, $W(V)$) is the width of the depletion layer with an applied bias of V volts and W_e is the width of the depletion edge region *i.e.* $W = \left[2\varepsilon_0\, \varepsilon\, (E_F - E_T)/e_n^2\right]$. Here, E_T is the trap depth, e_n is the emission rate from the trap, and other terms have their usual meanings.

3. Results and discussion

Three different groups of DLTS experimental data will be presented and analysed. These are: (a) DLTS of undoped GaN Schottky diode, (b) DLTS of lightly-doped GaN Schottky diode and (c) DLTS of moderately-doped GaN Schottky diode. Three experiments were performed on a few samples. For simplicity only one DLTS signal of a typical sample under t_1/t_2 = 75/225 is presented.

3.1 DLTS of undoped GaN Schottky diode :

DLTS spectrum of the undoped sample (Figure 2) shows two structures and exhibits negative values of ΔC, justifying the existence of two electron trap levels. A peak occurs at about 154 K, indicating the presence of a level. Let us call this level as L_1. Another peak in Figure 2 appears around 312 K. Let us call

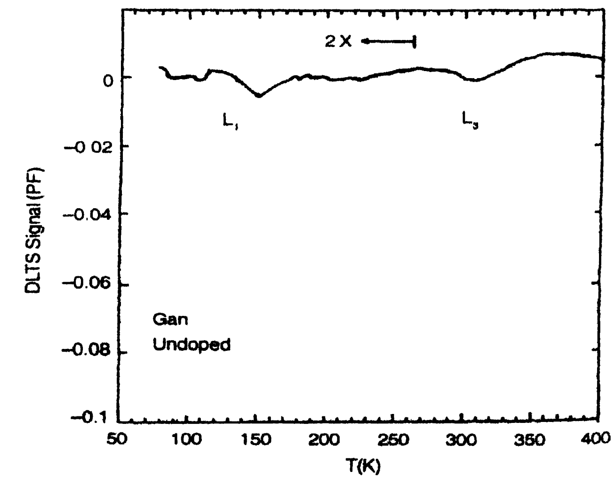

Figure 2. DLTS spectra of undoped GaN Schottky diode.

this level L_3. This peak is too weak to appear in a few undoped samples and is relatively broad when it appears weakly in some samples. The peak-shift towards the left in sequential order using different rate windows, is not prominent.

3.2 *DLTS of lightly doped GaN Schottky diode :*

Figure 3 shows the typical DLTS data of lightly-doped GaN Schottky diode using three different rate windows with a fixed value of t_1/t_2 = 1/3. For the case of spectrum S_1 : 75/225, three peaks at 154 K, around 200 K and at 312 K are observed and they show negative values of ΔC signifying the existence of electron trap levels. Similar peaks are also found in case of S_2 and S_3 spectra. Peaks corresponding to two single trap levels L_1 and L_3 are found to be shifted towards the left in sequential order. The peak that occurred at about 200 K is relatively broad. Let us call this level as L_2. This peak moves neither left nor right corresponding to the changing values of t_1/t_2 and rate windows, but the height of the peak varies widely corresponding to different rate windows even when the value of t_1/t_2 is kept constant. Thus, this peak disobeys sequential transient theory.

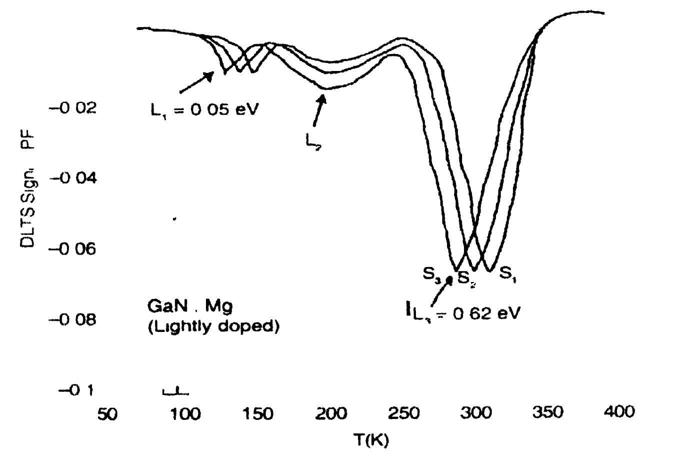

Figure 3. DLTS spectra of lightly-doped GaN Schottky diode where Mg is the dopant.

In addition, the variation of broadening and height of this peak have exhibited a very peculiar behaviour. It is therefore assumed that a number of trap levels exist around this temperature possibly forming a continuous distribution of states that occupy a certain energy level width rather than as single discrete level. Similar phenomenon in the study of DLTS of CdTe-ZnTe heterojunction was observed where the variation of broadening and peak height was attributed to be due to contributions of more than one deep levels [15].

The peak that appears at 154 K has been identified as level L_1. This peak has been observed to be shifted towards left corresponding to changing values of t_1/t_2 and rate windows *i.e.* it obeys sequential transient theory. The peak height of this sample is almost same compared to that of the undoped sample. Therefore, it is assumed that the origin of this level is due to unintentional dopant/impurity present in source materials and/or precursors in the growth of GaN.

The peak which has appeared in case of spectrum S_1 at 312 *K* is quite sharp. Let us identify this level as L_3 level. Similar peaks are also found in case of S_2 and S_3 spectra. The peak height of this level L_3 increases remarkably and is about one order more than that of the undoped sample. Therefore, this level L_3 is considered to be due to Mg dopant. Figure 4 shows the Arrhenius plot.

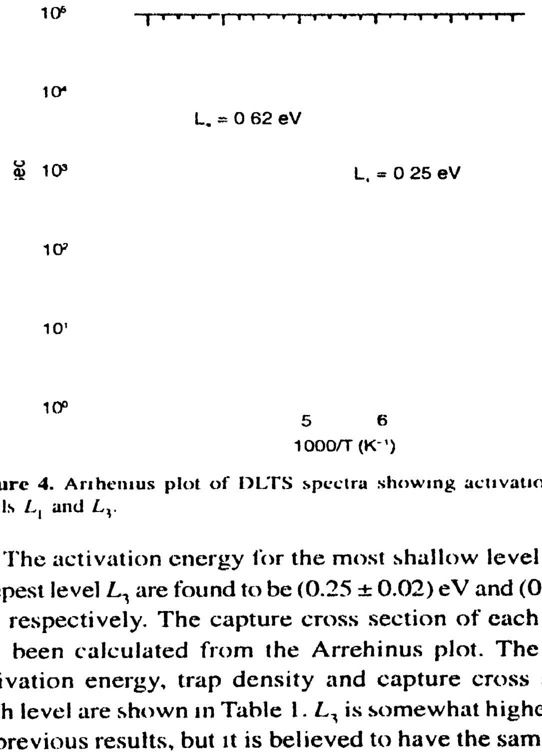

Figure 4. Arrhenius plot of DLTS spectra showing activation energy of levels L_1 and L_3.

The activation energy for the most shallow level L_1 and the deepest level L_3 are found to be (0.25 ± 0.02) eV and (0.62 ± 0.02) eV, respectively. The capture cross section of each trap level has been calculated from the Arrehinus plot. The values of activation energy, trap density and capture cross section of each level are shown in Table 1. L_3 is somewhat higher than that of previous results, but it is believed to have the same origin as reported to be 0.49 eV [16], 0.58 eV [17] and 0.44 eV [18], because of their similar patterns on an Arrehinus plot. Possible reasons for differences in measured energies include temperature differences between the sample and the measuring device and stress in the crystal.

Level L_3 was suggested not to be caused by Si by two separate studies [16, 17] since it occurs independently of whether or not Si is added. On the other hand, the level found at 0.665 eV in Hydride Vapour Phase Epitaxy (HVPE) grown [16] was not apparent in these tests or other tests employing Metal Organic Chemical Vapour Deposition (MOCVD) grown GaN [17, 19, 20]. This reveals the characteristics of the HVPE grown GaN. However, recent reports [21] from their study on the direct observation and electrical/optical characterization of the deep level spectrum show that the passivation of 0.62 eV level is consistent with Mg-H complex generation. From their argument, H-passivation of 0.62 eV suggests that point defects rather than threading dislocations are responsible for this level. This is what we have identified for this L_3 level as due to Mg dopant.

Theoretical studies reveal that N on Ga site may produce a deep level in the upper band gap region [22], but it is not an energetically favourable site for electron trap [23]. It has been suggested that a triplet of donor like states exist below the conduction band caused by V_N [24]. It is also reported that C on Ga site forms a level [22]. On the other hand, Lee *et al* [16] suggested that C may be responsible for a deep level of 0.14 eV. Our results from undoped samples show that despite the use of TMG, the concentration of these levels can be fairly minimized to the low range (10^{13} cm^{-3}).

3.3 DLTS of moderately doped GaN Schottky diode :

Figure 5 shows the typical DLTS data of moderately-doped GaN Schottky diode using three different rate windows with a fixed value of $t_1/t_2 = 1/3$; capacitances were measured at times t_1 and t_2. For the spectrum S_1 : 75/225 two peaks at 154 K and 312 K are observed. The negative values of ΔC signify the existence of two electron levels. Similar peaks are also found in the case of S_2 and S_3 spectra. The activation energy for the most shallow level L_1 is identical to those of undoped and lightly-doped GaN Schottky diodes. Surprisingly, the peak height does not depend on whether the sample is undoped, lightly-doped or moderately-doped GaN Schottky diode. This means that the concentration of this level is almost constant and is independent of doping concentration. Thus, the level L_1 is considered to be due to unintentional dopant/impurity presence in the grown GaN sample. Similar information regarding L_1 has been reported [25]. This level L_1 is also similar to that already reported [26] in films grown by different methods.

Detailed DLTS studies and theoretical fittings indicate that such trap is likely related to defects or defect-impurity complexes segregated around threading dislocations, that are typical in this GaN layers grown over sapphire substrates.

An energy level having activation energy of 0.62 eV which is the same for level L_3 from our DLTS studies, is previously identified with a trap [16-18] in undoped GaN films. This level was also reported [25] not only in undoped layers but also in weakly Mg-doped films. However, there is no discussion or any comment regarding the variation of peak height of this level between undoped and Mg-weakly doped films. In fact, this deep level is commonly labelled as E_2 in some literature. This level has also been observed in HVPE grown layer over sapphire [27] and free-standing samples and in undoped films grown by Molecular Beam Epitaxy (MBE) [28]. Although it is true that early studies [16] suggested that the centre could be due to chemical impurities like carbon (C), later capacitance transient spectroscopy investigations indicated a possible defect nature [29]. Another study showed that E_2 could be effectively suppressed of being N_{Ga} defect [30] which agrees with DLTS studies of GaN layers of different thickness [27]. These works also indicate that the trap E_2 is not related to N vacancies. The above discussion seems to be quite puzzling when we analyze our DLTS results regarding L_3, because the peak height of level L_3 increases remarkably and is two order higher than that of the undoped sample and one order higher than the lightly-doped sample. Therefore, there is little doubt to infer that this level L_3 is due to Mg-dopant. The L_3 peak observed in undoped sample was relatively broad and no occurrence of peak shift was observed. This is considered to be due to contamination of Cp_2Mg used as precursor in the growth chamber. Therefore, the level L_3 is attributed to Mg associated level. Figure 6 shows the comparative picture of typical DLTS of undoped, lightly-doped

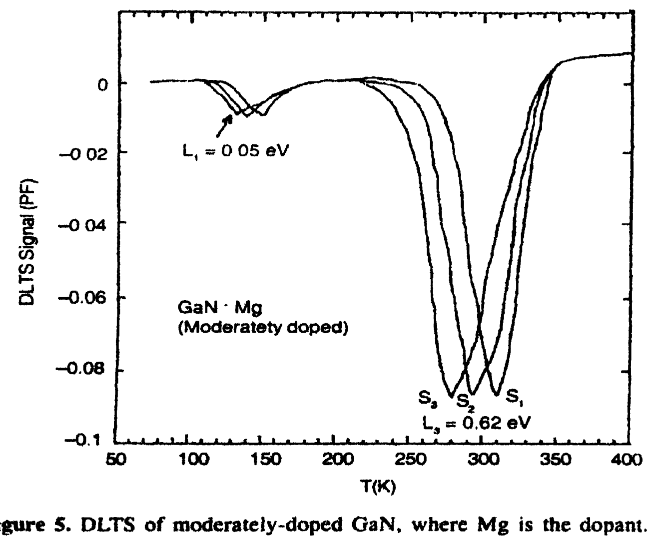

Figure 5. DLTS of moderately-doped GaN, where Mg is the dopant.

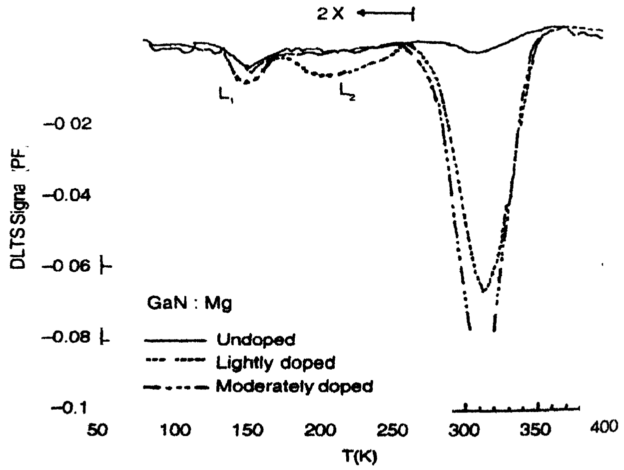

Figure 6. Comparative picture of typical DLTS spectra of undoped, lightly-doped and moderately-doped GaN, the dopant being Mg.

and moderately-doped GaN. The surprising aspect of Figure 6 is the absence of level L_2. L_2 does not appear in the undoped sample as well as moderately-doped sample whereas L_2 appears as a broad peak in case of lightly-doped sample. The origin of the level L_2 is not clear at this stage. The absence of L_2 in case of moderately-doped sample also remains explained.

4. Conclusion

The results of deep level studies of undoped, lightly-doped and moderately-doped GaN Schottky diode by DLTS are summarized as follows:

(a) Undoped GaN sample has a deep level $L_1 = (0.26 \pm 0.02)$ eV and is attributed to unintentional dopant/ impurity present in the grown sample. Another deep level $L_3 = (0.62 \pm 0.02)$ eV is too weak to appear in some samples and is relatively broad when it appears weakly.

(b) Lightly-doped GaN sample has deep levels L_1, L_2 and L_3. The behaviour and origin of L_1 level is considered to be similar to that of undoped sample. Level L_3 has the activation energy of (0.62 ± 0.02) eV. The origin of this L_3 is considered to be due to Mg-dopant from Cp_2Mg used as precursor. A broad peak at 180 K termed as L_2 level has been observed only in lightly-doped samples. From the variation and broadening and peak height of this peak, it is considered that L_2 is attributed to more than one deep level.

(c) Moderately-doped samples exhibit L_1 and L_3 levels. The origin of these levels are similar to that of undoped and lightly-doped samples.

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